**Computational Toxicology—Objective 2: Developing Approaches for Prioritizing Chemicals for Subsequent Screening and Testing**

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One of the strategic objectives of the Computational Toxicology Program is to develop approaches for prioritizing chemicals for subsequent screening and testing. Approaches currently available for this process require extensive resources. Therefore, less costly and time-extensive computational approaches must be developed to determine which chemicals or classes of chemicals should be screened and tested first. Three areas in which computational approaches will substantially impact on the prioritization process include quantitative structure-activity relationships (QSARs) and other computational approaches, pollution prevention strategies, and high-throughput screening. QSARs have been used to optimize laboratory testing, provide estimates of missing data in lower-tier risk assessment, and estimate the toxicity of untested chemicals directly from chemical structure. Emerging "omics" technologies have excellent potential to generate information that will inform and improve the QSAR modeling process. In support of pollution prevention strategies, ORD is developing methods to estimate the potential environmental impact of chemicals that are released into the environment. These methods are used to evaluate chemicals for potential harm both to humans and the environment in a life-cycle assessment framework. Regardless of the level of sophistication in the models, the final impact indicators (e.g., a broad range of midpoint effects or final outcomes, such as human deaths, human illnesses, crop damage, water quality issues, and air quality issues) could be used to compare a large number of chemicals. Applications of new molecular and other technological advances hold promise for the development of high-throughput screens (HTPS). For example, new approaches have the potential for making significant advances over existing screens for endocrine-disrupting chemicals (EDCs) in terms of speed, high-throughput capability, sensitivity, reproducibility, and reduction in animal usage in a screening and testing program.